Comparison of Two Techniques to Develop Pedotransfer Functions for Water Retention

J. Tomasella,* Ya. Pachepsky, S. Crestana, and W. J. Rawls

ABSTRACT

Two pedotransfer function (PTF) approaches can be used for obtaining the analytical expression of the whole retention curve: (i) soil basic data is used to estimate soil water retention at specific water potentials; and then an analytical expression of the retention curve is fitted to the estimated soil moisture values; and (ii) soil basic data is used for estimating the parameters of an analytical expression of water retention curves. The objective of this study was to compare the performance of both techniques using data representing the main Brazilian soils. First, we derived PTFs for the parameters of van Genuchten equation and for water contents at -6, -10, -33, -100, and -1500 kPa for the same development data set. Second, we compared the performance of both techniques for the same validation data set. The approach, based on the estimation of water contents at specific water potentials, provided better results: for the validation data set, this technique showed an average root mean squared error of 0.036 m^3 m^{-3}, compared with an averaged error of 0.098 m^3 m^{-3} of the technique based on the direct estimation of van Genuchten parameters. A possible explanation for this result might be related to the fact that soil moisture is controlled by different independent variables at different ranges of soil water potential, and those differences are not directly related to the van Genuchten parameters.

K NOWLEDGE OF soil hydraulic properties is needed for many applications in hydrology, agronomy, meteorology, ecology, and environmental protection. During a preliminary design of research on small plots, or in large project areas where measurements are impractical (Carter and Bentley, 1991), soil hydraulic properties need to be estimated by the use of PTFs. The term *pedotransfer function* was first introduced for empirical regression equations relating water and solute transport parameters to the basic soil properties that are available in soil surveys (Bouma, 1989). Developing PTFs is a growing field, as seen in recent reviews (Rawls et al., 1991; van Genuchten and Leij, 1992; Pachepsky et al., 1999; Wösten et al., 2001).

The soil water retention curve, one of the hydraulic properties often estimated with PTFs, describes the dependence of soil water content on soil water potential. This dependence is usually represented by an analytical equation, with a small number of parameters. The water retention equation is fitted to soil water retention measurements adjusting its parameters to match, as close as possible, measured water retention values. Therefore, the parameters control position and shape of the water retention equation.

If both soil basic data and soil water retention information are available for a set of samples, two approaches can be used to estimate the relationship between the parameters of an analytical equation of soil water retention and soil basic data: (i) fit the parameters of the analytical equation to measured values for each sample of the data set; (ii) build a table relating those parameters to their corresponding soil basic data; and (iii) develop a relationship between fitted parameters and soil basic data. The second approach is: (i) build a relationship between water contents at selected soil water potentials and soil basic data; and (ii) fit the parameters of the analytical water retention equation to the estimated water contents. In other words, the first approach fits the analytical curve first, and uses PTF estimations later, whereas the second approach uses PTF estimation first and fits the analytical curve later.

Both approaches have been widely used for various databases. The first approach, referred to as the *parametric* in this paper, has been used in the PTFs development, for instance, by Vereecken et al. (1989), Schaap et al. (1998), Minasny et al. (1999), and Wösten et al. (2001). The second technique, referred to as the *point-based* in this paper, was used in PTFs developed by Baumer (1992). For Brazilian soils, point-based PTFs have been developed by Tomasella and Hodnett (1998) and by van den Berg et al. (1997). More recently, Tomasella et al. (2000) developed a PTF based on the parametric approach.

There are indications that the parametric approach may lead to lower accuracy in water retention predictions compared with the point-based approach. Reasons for that may be (i) soil water retention in different ranges of soil water potential is affected by different basic soil properties (Visser, 1969), and (ii) coefficients obtained from fitting the retention equation to data may have low reliability due to the inherent correlation between those coefficients or due to nonuniform distribution of soil water potential levels at which the water retention was measured (Vereecken et al., 1989; Scheinost et al., 1997). On the other hand, Vereecken et al. (1992) have argued that parametric technique (i) facilitates efficient comparisons among soils, and (ii) the dependent variable does not have to be measured at prespecified levels of soil water potential. This is, indeed, important if water retention data are coming from vari-

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ous laboratories in which different soil water potentials were used.

The performance of PTFs, either based on the parametric or point-based approach, is usually analyzed comparing the quality of the estimations when applied on a particular soil data set (Schaap and Leij, 1998). It is important to note, however, that those PTFs were developed from different data sets, and their predictive ability is somewhat related to the similarity between the data set used in the developing and testing of the PTF (Tomasella et al., 2000).

However, we are not aware of any study comparing the accuracy of the parametric and point-based techniques when developed and tested using the same data set. Therefore, the objective of this study was to compare parametric and point-based approaches to develop PTFs for soil water retention using a comprehensive database on water retention of Brazilian soils.

MATERIALS AND METHODS

We used the database of Tomasella et al. (2000), augmented with new data to represent a greater variety of Brazilian soil types (Fig. 1). Since water retention is not standard information in Brazilian soil surveys, Tomasella et al. (2000) selected

data coming from different sources, resulting in 838 measured water release curves.

Physical and chemical properties were determined using the methodology recommended in EMBRAPA's (1997) soil survey manual. Basic soil properties included four texture fractions: coarse sand (2–0.2 mm), fine sand (0.2–0.05 mm), silt (0.05–0.002 mm), and clay (<0.002 mm); organic C content, moisture equivalent, and bulk density. Water release data were obtained from undisturbed soil cores (minimum internal volume of 50 cm^2) using the same methodology: tension tables between saturation and −10 kPa, and pressure chambers between −10 kPa and −1500 kPa. Bulk density was determined after drying soil cores at 105°C for 24 h, and particle density (when available) by volumetric flask. Porosity was derived from the bulk density and particle density. The pipette method was used to determine silt and clay fraction, sand fractions were separated by dry sieving. Organic C was estimated by wet digestion with acid dichromate automatic titration in iron sulfate. Organic C is usually correlated with organic matter in Brazilian soils. For this reason, EMBRAPA's (1997) soil survey manual recommends to derive organic matter assuming that organic C constitutes about 58% of the mean composition of humus. For this reason, we selected organic C, a direct measured variable, rather than organic matter, as an independent variable in the PTF. Finally, moisture equivalent was determined as the gravimetric moisture content remaining in a disturbed soil sample after centrifuging at 2400 rpm for 30 min.
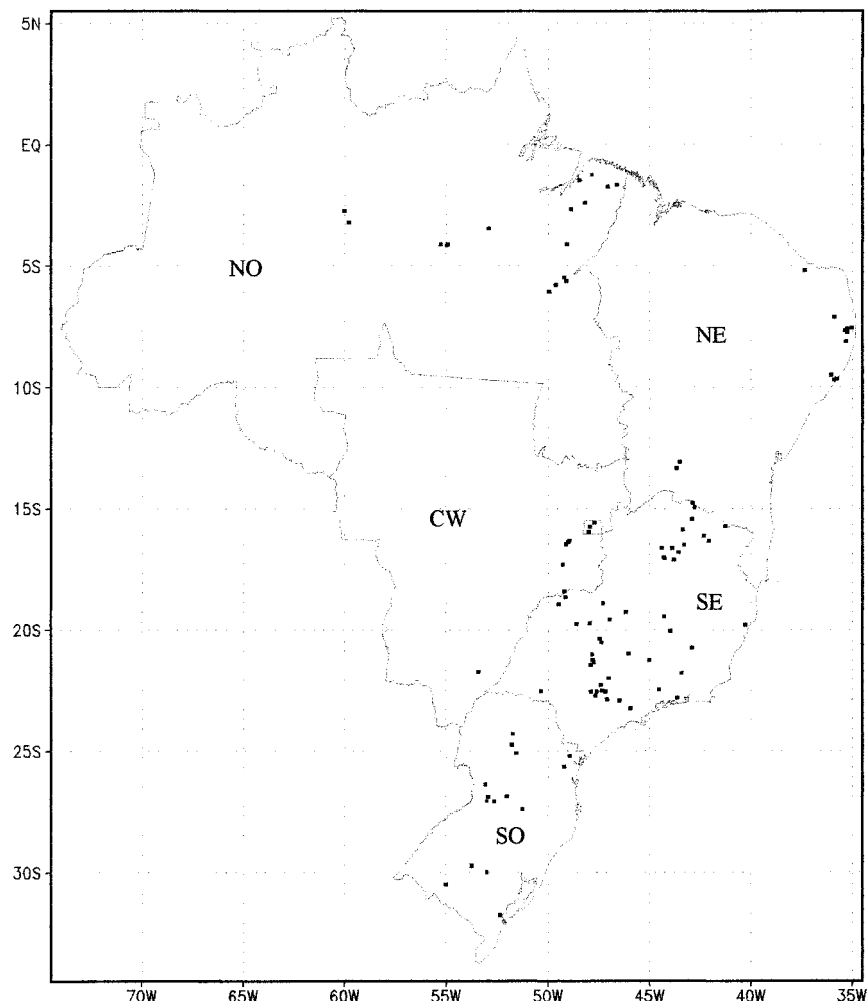

Fig. 1. Geographic domain where soil water retention data was available for this work. The map also shows the main geographical regions of Brazil, namely SO–South, SE–Southeast, CW–Center West, NE–Northeast, and NO–North.

Since soil retention data came from different sources, only those samples defined by at least five pairs of water retention points were included in the database (Tomasella et al., 2000). This minimum was arbitrary selected because analytical retention curves commonly used have four or less parameters. To derive PTFs with parametric and point-based approaches, the following steps were taken.

Step 1. Soil retention data for the 838 samples available in the database were fitted to the analytical equation proposed by van Genuchten (1980):

$$\theta = \frac{\theta_0 - \theta_r}{[1 + (\alpha|h|)^n]^{1-1/n}} + \theta_r, \qquad [1]$$

where θ is the volumetric water content [$m^3 \, m^{-3}$], h is the water potential [kPa]; θ_0 is the saturated water content, θ_r is the residual water contents, α and n are parameters governing position and shape of the water retention curve. In this study, van Genuchten parameters θ_0, θ_t, α, and n were estimated using the RETC code for quantifying the hydraulic conductivity of unsaturated soils (van Genuchten et al., 1991).

Step 2. We created a homogeneous data set to be used in the point-based method. Since the number of points and the specific water potentials differed between data sources, water potential values selected for developing PTFs for the point-based approach were: zero, −6 kPa, −10 kPa, −33 kPa, −100 kPa, and −1500 kPa. Moisture contents at those potentials were measured in all available curves, except for the moisture content at −6 kPa water potential that was not measured in 43% of the total number of water release curves. Therefore, the point-based equation for −6 kPa water potential was derived and validated from 477 data-points, compared with a total of 838 data points used on other potentials. Porosity was assumed to be equal to water content at saturation, and was derived from bulk and particle densities. Since some sources did not provide particle density data, the porosity was not available on nine of the 838 water release data available, and only 829 data points were used in the derivation and validation for porosity.

Step 3. The development and testing data sets were created. First, the whole dataset was subdivided into regional databases. This strategy was adopted since Brazil has a wide variety of climate, vegetation, and geological environments, and pedogenetic processes are quite different along the country. Brazil is divided in five regions (Fig. 1): the Northeast, which is broadly speaking semiarid; the North, covered by the tropical rainforest; the South, which is a more temperate environment; the Center-West, mainly dominated by the *cerrado* (savanna); and the Southeast, which is a transition between the savanna and a temperate climate. Second, each regional dataset was split randomly into development (75%) and testing (25%) regional subsets. Finally, regional development (testing) data sets were combined in one national development (testing) data set. This procedure ensured that both development and testing data sets cover all country regions.

Step 4. The PTF equations were derived relating (i) water contents at selected water potential to soil basic data for the point-based approach, and (ii) the van Genuchten parameters to soil basic data for the parametric approach.

The group method of data handling (GMDH) was used to develop the PTF equation. The GMDH is a heuristic, neuronet type regression technique that retains only essential input variables in a flexible net of polynomial regression equations (Farrow, 1984). The GMDH provides an automated selection of essential input variables and builds hierarchical polynomial regressions, usually with fewer nodes than artificial neural networks. More details about the application of the GMDH

for PTF development can be found in Pachepsky and Rawls (1999) and Pachepsky et al. (1998). The version of the GMDH used in this paper is coded in the commercial software ModelQuest (AbTech Corp, 1996), that uses the following predicted squared error criteria, PSE:

$$PSE = SSE + CM(2k/T), \qquad [2]$$

where SSE is the sum of squared errors, CM is the complexity penalty multiplier, k is the number of terms in the network model, T is the number of training observations. The value of CM is found by optimization so that the model with smallest number of nodes is found to provide the minimum absolute error. The development data set was used to derive the PTFs.

Step 5. The PTF from the point-based method was used to compute water contents at selected potentials in the testing data set, then van Genuchten equation parameters were fitted to computed water contents for each sample, and subsequently, water contents at the selected potentials were computed with this equation. The PTF from the parametric approach was also applied in the testing data set to estimate van Genuchten parameters from basic soil properties, and then water contents at the selected potentials were estimated from this equation.

Step 6. For individual water contents, the accuracy for the two approaches was compared using the root mean squared error, RMSE:

$$RMSE = \frac{(\theta_m - \theta_p)^2}{ND}, \qquad [3]$$

where the subscripts m and p indicate predicted and measured soil moisture values, respectively, and ND is the number of data points.

For comparing water retention curves, the root mean squared difference, RMSD, (Tietje and Tapkenhinrichs, 1993) was used:

$$RMSD = \sqrt{\frac{1}{d - c} \int_c^d (\theta_m - \theta_p)^2 \, dh}, \qquad [4]$$

where c and d define the integration interval. As suggested by Tietje and Tapkenhinrichs (1993), the integrals were calculated using $\log_{10}(h)$, and for this reason porosity was assumed to correspond to water the content at a potential of −0.01 kPa. Since the RMSD is an integrated statistic that takes into account the whole range of water potentials, it is useful to exam if point-based estimations provide accurate estimations of individual water content but fail in reproducing the shape of the retention curve. Performances between both techniques were tested using the F statistics, as suggested by Rajkai et al. (1996).

RESULTS

The t test for both the development and validation data demonstrated that the groups were not significantly different (Table 1). Except for the fine sand values, all values from testing data set were within the ranges found in the development data set. The texture distribution in both the development and validation data sets is typical for Brazilian soils (Fig. 2), since they are usually clayey, low-density, kaolinitic, with relatively low silt content varying between 10-20%, and rarely exceeding 40%. As was noted by Tomasella et al. (2000), most Brazilian tropical soils are quite different in terms of texture characteristics, with strong implications on soil

Table 1. Statistics of variables used on the development and validation of the pedotransfer function. Ranges of soil texture correspond to the USDA classification.

Statistics	Coarse sand	Fine sand	Silt	Clay	Organic C	Moisture equivalent	Bulk density
			%			g g^{-1}	g cm^{-3}
				Development			
Mean	19.92	14.54	16.29	49.25	0.95	0.25	1.25
SD	18.65	12.37	15.37	23.38	0.85	0.11	0.21
Max.	74.60	65.00	71.00	96.00	6.39	0.53	1.91
Min.	0.00	0.00	0.00	1.70	0.00	0.02	0.72
				Validation			
Mean	15.76	13.37	21.44	49.42	1.33	0.28	1.19
SD	16.77	15.91	14.52	20.14	0.99	0.13	0.22
Max.	76.00	72.00	67.00	79.38	4.18	0.55	1.65
Min.	0.00	0.00	1.00	7.00	0.22	0.03	0.72

water behavior, compared with soils of temperate climate. For a quick comparison, see for instance Fig. 1 of Tiejte and Tapkenhinrichs (1993) or Fig. 1 of Schaap and Leij (1998).

The van Genuchten equation fitted Brazilian water retention data with high accuracy (Table 2), similar in quality with the fittings of Schaap et al. (1998). These results clearly indicate that the van Genuchten equation was suitable for fitting water retention data of Brazilian soils.

PTFs developed with the GMDH for point-based and parametric methods are given in the Appendix. The four fractions of texture, organic C, and moisture equivalent were used as predictors in the development of the PTFs (Table 3). We also tried to use the cation exchange capacity as a predictor but did not find a significant improvement (data not shown). Coarser texture fractions served as predictors for high water potential, whereas fine fractions worked as predictors at low (large negative) potentials. The absolute error of the estimation decreased as the water potential decreases. With the parametric method, the estimates were reasonably accurate for the θ_0 parameter and slightly less accurate for the θ_r parameter. Predictors of θ_0 were the same as those used for porosity, and the accuracy of the estimation was very similar for both. Estimation of log α and log n resulted in R^2 much lower than the estimation of θ_0 and θ_r. The list of predictors in the final equation for α suggests that its value was affected by a combination of independent variables that control the moisture values at both high and low water potentials. Values of n appeared to be controlled mainly by the bulk density and the moisture equivalent.

The application of the point-based PTF showed a

similar agreement between observed and estimated moisture content in both the testing and the development data sets (Table 4). On the other hand, the accuracy of the PTF based on the parametric technique to the testing data set was substantially lower compared with the development data set (Table 4). The performance of the point-based technique was superior at all levels of soil water potentials and for integrated water retention curves (Table 4).

DISCUSSION

Application of two methods to estimate soil water retention gave strikingly different results, even though the equation to fit water retention curves and soil survey data used as predictors were the same for both methods. Accuracy of each method with Brazilian data set was similar to the accuracy of that method applied to other data sets. For example, Ahuja et al. (1985) applied the point-based estimation to the Southern plain database and obtained the accuracy of about 0.05 m^3 m^{-3}. Schaap and Leij (1998) applied the parametric estimation method to three databases and obtained overall RMSE of $\approx$0.1 m^3 m^{-3}. These values are close to the values in Table 4.

Data in Table 3 indicate that the coarse-textured fractions affect water contents near saturation, and fine fractions were more relevant at lower moisture content. Similar results were found with other soil hydraulic databases (Rawls et al., 1991).

Organic C was not selected by the GMDH algorithm to be an essential input variable in PTFs, although it was presented in the list of possible inputs for the GMDH to build PTFs. One possible reason is that not only quantity
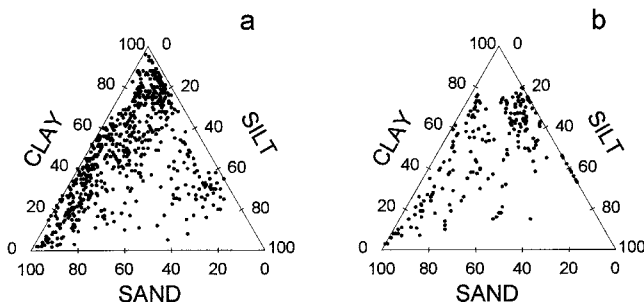
Fig. 2. Texture of samples in the development and testing soil data sets in this study.

Table 2. Accuracy of the van Genuchten equation fitted to the water retention data for the complete data set in terms of the root mean squared difference, RMSD (value in parenthesis), and the root mean squared error, RMSE.

Variable	(RMSD)/RMSE
	m^3 m^{-3}
Retention curve	(0.013)
Porosity	0.003
−6 kPa	0.008
−10 kPa	0.006
−33 kPa	0.009
−100 kPa	0.010
−1500 kPa	0.007

Table 3. Performance of the pedotransfer functions developed with the group method of data handling algorithm in terms of the root mean squared error, RMSE, and the determination coefficient, R^2.

Variable	Development data set		Testing data set		Predictors¶
	RMSE	R^2	RMSE	R^2	
	Point-based approach				
0 kPa	0.040	0.915	0.042	0.887	CS, S, D_b
−6 kPa	0.035	0.954	0.046	0.892	CS, S, Me, D_b
−10 kPa	0.031	0.960	0.037	0.958	S, Me, D_b
−33 kPa	0.021	0.979	0.024	0.982	Me, D_b
−100 kPa	0.020	0.977	0.030	0.958	C, Me, D_b
−1500 kPa	0.025	0.955	0.037	0.938	C, Me, D_b
	Parameter-based approach				
θ_0	0.040	0.917	0.039	0.905	CS, S, D_b
θ_r	0.062	0.791	0.111	0.461	S, Me
$Log_{10}\ \alpha$	0.630	0.602	0.951	0.404	CS, FS, S, C, Me, D_b
$Log_{10}\ n$	0.068	0.526	0.097	0.345	CS, Me, D_b

¶ CS, coarse sand content; FS, fine sand content; S, silt content; C, clay content; Me, moisture equivalent; D_b, dry bulk density.

but also quality of organic matter content affects soil water retention. Rawls et al. (2003) compared relative effects of organic matter on water retention using PTFs developed in different regions, and found large regional differences. Our database encompasses several regions with vastly different combinations of soil-forming factors. Another reason may be that the moisture equivalent and bulk density together make the use of organic matter in PTFs unnecessary. We may have encountered the same situation as Bloemen (1980), who has demonstrated that bulk density effectively substituted organic matter content in PTF development with his data set.

Variations in accuracy in Table 4 can be partly explained by the inability of PTFs in capturing differences in structure using the set of predictors that we had. The low accuracy of the van Genuchten parameter estimates with this type of predictors has been observed with other soil hydraulic databases (Pachepsky et al., 1996; Schaap et al., 1998). It is possible that those parameters reflect soil structure rather than soil texture. The importance of structure for water retention of Brazilian soils is supported by the fact that both bulk density and moisture equivalent, which are indirect indications of structure, appears in the point-based equations at all soil water potentials. Descriptions of soil structure can be found in soil survey databases, but these descriptions are given in categorical rather than in numerical form. Using categorical structural data to estimate van Genuchten's parameters presents an interesting issue to explore, considering that van Genuchten's equation showed an excellent performance for fitting water retention data of

Brazilian soils (Tables 2, 4). Recently Rawls and Pachepsky (2002) have applied regression tree technique to NRCS database and have shown that using categorical information about soil structure can improve estimates of water retention.

One reason for the significance of structure for hydraulic properties of Brazilian soils may be the relatively low content of silt fraction as compared with soils from the temperate climate regions. The domination of very coarse and very fine particles over particles of the intermediate sizes makes the particle packing patterns very important for hydraulic properties. We note that such features in texture can be found in other tropical soils (MacLean and Yager, 1972; Babalola, 1978).

Several factors could contribute in the superiority of the point over the parametric method in this work. The difference in data used could not contribute since the same dataset has been used to calibrate and validate both methods, and both point and parametric data were optimized using sum of squared differences between measured and simulated water contents. It is theoretically possible (but hardly probable) that regression-based GMDH method would perform better on point data than on parametric data.

It is well known that a group of basic soil properties are more important in the wet range of the water retention curve, while other properties control the variability on the dry range. Shape parameters of the analytical water retention curve, on the other hand, describe its behavior both in the dry and wet range. Therefore, the most probable explanation for a better performance

Table 4. Performance of point-based and parametric water retention estimation for the development and testing data set.

Statistic	Development data set			Testing data set		
	Point-based	Parametric	F value	Point-based	Parametric	F value
RMSD†	0.087**	0.182**	2.021	0.087**	0.206**	2.271
RMSE‡ (porosity)	0.040	0.116	1.008	0.042	0.039	0.927
RMSE (−6 kPa)	0.035**	0.111**	3.311	0.046**	0.129**	2.831
RMSE (−10 kPa)	0.031**	0.092**	3.621	0.037**	0.125**	3.353
RMSE (−33 kPa)	0.021**	0.075**	4.390	0.024**	0.113**	4.621
RMSE (−100 kPa)	0.020**	0.055**	3.692	0.030**	0.102**	3.370
RMSE (−1500 kPa)	0.025**	0.182**	2.173	0.037**	0.079**	2.118

** According to the Fisher test, the sum of squared errors at the same potential for the point-based and parametric techniques are statistically different at $P < 0.01$.
† RMSD, root mean squared difference.
‡ RMSE, root mean squared error.

of the point over the parametric method is that the relationship between water retention parameters and basic soil properties is highly complex and cannot be accurate described by the parametric method.

We note that Schaap and Bouten (1996) made a similar comparison and did not observe such large differences between two methods. However, their database consisted mostly of coarse soils, whereas our database contained soils with wide range of textures. Minasny et al. (1999) also made a similar comparison and saw the need in improving of parameter estimates by refitting the van Genuchten equation to actual data points.

CONCLUSIONS

Overall, the point-based method was superior to the parametric method of PTF development for Brazilian soils. This might be explained by the fact that moisture content is controlled by different independent variables at different water potentials in Brazilian soils, and the PTF developed for point-based method allows for a more appropriate combination of those independent variables. The PTF developed for the parametric approach, particularly for the estimations of the parameters log α and log n, needs to take into account the whole range of soil water potentials, and the relationships between the parameters and the independent variables are apparently not straightforward. Further comparisons are necessary to determine whether this conclusion holds for soil from regions with temperate climate.

ACKNOWLEDGMENTS

APPENDIX: ALGORITHMS TO ESTIMATE VAN GENUCHTEN'S PARAMETERS AND VOLUMETRIC WATER CONTENT AT SELECTED SOIL WATER POTENTIALS

Symbols: CS, coarse sand (%); FS, fine sand (%); S, silt (%); C, clay (%); D_b, bulk density (g cm^{-3}); Me, moisture equivalent (%); θ_0, α, n, and θr, parameters in the van Genuchten equation; θ_0, θ_6, θ_{10}, θ_{33}, θ_{100}, and θ_{1500}, volumetric water contents at 0, 6, 10, 33, 100, and 1500 kPa, respectively; x_1–x_{17}, and z_1–z_{13}, auxiliary variables.

GMDH-Generated Algorithms

$$x_1 = -1.0679 + 0.0536107 \times CS$$
$$x_2 = -1.17468 + 0.0808098 \times FS$$
$$x_3 = -1.05976 + 0.0650437 \times S$$
$$x_4 = -2.10641 + 0.0427715 \times C$$
$$x_5 = -2.21391 + 8.92268 \times Me$$

$$x_6 = -6.03516 + 4.81197 \times D_b$$
$$z_1 = 4.25417x_1 + 2.72322x_2 + 3.07242x_3$$
$$+ 5.00093x_4 - 0.195062x_5 - 0.377081x_6$$
$$z_2 = 0.110144 + 0.640373z_1 - 1.16884(z_1)^2$$
$$- 0.155394x_4 - 0.358591z_1x_4$$
$$- 1.00996(z_1)^2x_4 + 0.126617\ (x_4)^3$$
$$\alpha = 10^{\ 0.0736768\ +\ 0.789068z_2}$$
$$z_3 = 0.37398x_1 - 0.0940338(x_1)^3 + 0.838535x_1x_5$$
$$- 0.590525\ (x_1)^2x_5 + 0.76113\ (x_5)^2$$
$$- 0.789465x_1(x_5)^2 - 0.273647(x_5)^3$$
$$- 0.512764x_6 + 0.455363x_1x_6 - 0.38428(x_1)^2x_6$$
$$+ 0.731809x_5x_6 - 1.00484x_1x_5x_6 - 0.172341(x_5)^2x_6$$
$$+ 0.219746(x_6)^2 - 0.367679x_1(x_6)^2 + 0.131251(x_6)^3$$
$$z_4 = -0.360294 + 0.76878z_3 + 0.0770122(z_3)^3$$
$$- 0.193142x_2 - 0.121583z_3x_2$$
$$+ 0.0889415(z_3)^2x_2 + 0.284168(x_2)^2$$
$$- 0.0674767(x_2)^3 - 0.202897x_3 - 0.341951z_3x_3$$
$$- 0.270616x_2x_3 + 0.0880845(x_2)^2x_3 + 0.24982(x_3)^2$$
$$+ 0.102658x_2(x_3)^2 - 0.0801841(x_3)^3$$
$$n = 10^{\ 0.140543\ +\ 0.0797516z_4}$$
$$z_5 = 0.164417 + 0.126139\ (x_1)^2 + 0.281797x_3$$
$$+ 0.484823x_1x_3 - 0.293866\ (x_3)^2$$
$$- 0.354924x_1\ (x_3)^2 - 0.705803x_6$$
$$- 0.189153x_3x_6 - 0.267997x_1x_3x_6$$
$$- 0.023954\ (x_3)^2x_6 - 0.0918816x_1(x_6)^2$$
$$+ 0.0323997(x_6)^3$$
$$\theta_0 = 0.515224 + 0.100899z_5$$
$$z_6 = 0.12867 - 0.492412x_3 + 0.787425x_5$$
$$- 0.235254x_3x_5;$$
$$\theta_r = 0.161487 + 0.101111 \times z_6$$
$$x_7 = -1.0553 + 0.0533922 \times CS$$
$$x_8 = -1.07131 + 0.0649731 \times S$$
$$x_9 = -6.18145\ + 4.95385 \times D_b$$
$$z_7 = 0.159379 + 0.137397(x_7)^2 + 0.265398x_8$$
$$+ 0.519965x_7x_8 - 0.276027(x_8)^2 - 0.362393x_7(x_8)^2$$
$$- 0.702969x_9 - 0.222252x_8x_9 - 0.244634x_7x_8x_9$$
$$- 0.092267x_7(x_9)^2 + 0.0332669(x_9)^3$$
$$\theta_0 = 0.517589 + 0.0994301z_7$$
$$x_{10} = -1.17152 + 0.0500892 \times CS$$
$$x_{11} = -0.867548 + 0.0519417 \times S$$
$$x_{12} = -1.97975 + 8.3484 \times Me$$
$$x_{13} = -5.72537 + 4.53135 \times D_b$$

$$z_8 = -0.259878 \times x_{10} + 0.0867921 \times x_{11}$$
$$+ 0.806806 \times x_{12} + 0.196837 \times x_{13}$$

$$\theta_6 = 0.34505 + 0.117162z_8$$

$$x_{14} = -1.05501 + 0.0650857 \times S$$

$$x_{15} = -2.07588 + 0.0423954 \times C$$

$$x_{16} = -6.03402 + 4.80572 \times D_b$$

$$x_{17} = -2.18409 + 8.84963 \times Me$$

$$z_9 = 0.175202 + 1.18513 \times x_{17} - 0.0996042 \times (x_{17})^2$$
$$+ 0.327915 \times x_{16} - 0.0758657 \text{ x } (x_{16})^2$$

$$z_{10} = 0.929344 \times z_9 + 0.132519 \times x_{14}$$

$$\theta_{10} = 0.339255 + 0.112526 \times z_{10}$$

$$z_{11} = 0.191452 + 1.25652x_{17} - 0.079098(x_{17})^2$$
$$+ 0.393814x_{16} + 0.152095x_{17}x_{16}$$

$$\theta_{33} = 0.28951 + 0.103815z_{11}$$

$$z_{12} = 0.231205 - 0.0968656 (x_{15})^2 + 0.0799528 (x_{15})^3$$
$$+ 1.28868x_{17} + 0.13082x_{15}x_{17} - 0.143115 (x_{17})^2$$
$$- 0.126294x_{15}(x_{17})^2 + 0.429792x_{16}$$
$$+ 0.133537x_{17}x_{16} - 0.0661431x_{15}x_{17}x_{16}$$

$$\theta_{100} = 0.257093 + 0.0952908z_{12}$$

$$z_{13} = 0.235084 + 0.33033 \times x_{15} - 0.191838$$
$$\times (x_{15})^2 + 0.0543679 \times (x_{15})^3 + 0.977685$$
$$\times x_{17} + 0.304174 \times x_{15} \times x_{17} - 0.218857$$
$$\times (x_{17})^2 - 0.164373 \times x_{15} \times (x_{17})^2 + 0.0415057$$
$$\times (x_{17})^3 + 0.373361 \times x_{16} + 0.0811861$$
$$\times x_{17} \times x_{16} - 0.0768087 \times x_{15} \times x_{17} \times x_{16}$$

$$\theta_{1500} = 0.214008 + 0.0862945 \times z_{13}$$

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